CONTRIBUTION TO THE OPTIMIZATION OF EPITAXIAL GROWTH OF NITRIDE SEMICONDUCTORS: WHAT WE CAN LEARN FROM BASIC INTERFACE PHYSICS

P. Masri

Groupe d'Etude des Semi-conducteurs, CNRS-UMR5650, Université Montpellier 2, cc 074, 12 Place E. Bataillon, F-34095 Montpellier cedex 5, France
e-mail: masri@int1.univ-montp2.fr

Modern crystal-growth techniques can now afford a wide panoply of heterosystems for applied physics purposes. A comprehensive understanding of the problems involved in growth experiments implies the macroscopic and microscopic aspects of interface physics. Although the latter aspect is relevant to the very first stages of the growth process, the first aspect (of heteroepitaxy) must be taken into account because not only local features but also periodic and long-range features can influence the process. This is for example the case of Lomer dislocations which may be created at the interface between two host materials with mismatched lattice parameters when the overlayer thickness exceeds a critical value. An energy balance between strain-associated elastic energy and dislocation formation energy determines the overlayer critical thickness beyond which misfit dislocations (MD's) are energetically more favored than strains.

The lattice misfit between two materials A and B is related to the difference between their lattice parameters $\Delta=|a_A-a_B|$. The dislocations which are created when the conditions of strain relief are fulfilled are characterized by a geometric feature, namely the associated Burgers vector. At a nanometric scale, the elementary quantity which we may define is a “small” Burgers vector $b_e=a_B-a_A$, with $a_B>a_A$: b_e represents a rather small fraction of the lattice parameters. In the case of perfect epitaxy, b_e corresponds to small epitaxial dislocations. By a vernier effect, we end up with a network of epitaxial MD's which are fairly parallel with a lattice spacing equal to L. Their density is low when Δ is small: if $b_e \to 0$, one may expect that $L\to\infty$, ensuring a very small dislocation density. The appearance of the MD's corresponds to a negative free energy associated with these defects, as they aim at relaxing interface strains. The lattice spacing L is usually obtained by applying the following geometric conditions [1]:

$$(n_1+1)a_A=n_1a_B\ ;\ \ n_1=a_A(a_B-a_A)^{-1}\ ,\ \text{if}\ a_A<a_B \tag{1}$$
$$(n_1+1)a_B=n_1a_A\ ;\ \ n_1=a_B(a_A-a_B)^{-1}\ ,\ \text{if}\ a_A>a_B \tag{2}$$

If we consider , e.g., Eq. 1, it states that after n_1 jumps on the lattice B and (n_1+1) jumps on the lattice A, we may find in coincidence two interface sites belonging respectively to A and B. In the framework of the geometric approach L is then calculated by using the value of n_1 and the expression of the corresponding Burgers vector. Within this approach, we can learn that the best host materials for heteroepitaxy are those providing the highest value of L, i.e., eventually the lowest MD density.

In what follows, we will show that not only the geometric features of host materials are relevant to heteroepitaxy but also those features related to their elastic properties, through which the temperature effects are also involved as these elastic features are temperature dependent. The idea of taking account of these elastic features can be derived by analyzing the elasticity theory equations [2]. These equations relate strain to lattice dynamics features through relationships involving the $S=f(C_{ij})/\rho$ factor, where ρ is the density. For each interface configuration, i.e., for a specific growth plane, the dynamics equations involve effective elastic constants $f(C_{ij})$ which correspond to elastic waves propagating along the principal symmetry directions in cubic crystals. The expressions of $f(C_{ij})$ for the longitudinal and transverse modes are given below respectively for the [100], [110] and [111] principal directions:

- For longitudinal modes:

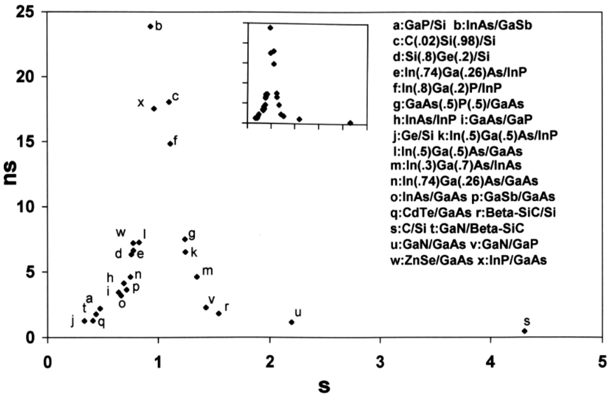
$$f(C_{ij})=C_{11}\ \text{(a)},\ f(C_{ij})=C_{11}+C_{12}+2C_{44}\ \text{(b)},\ f(C_{ij})=C_{11}+2C_{12}+4C_{44}\ \text{(c)} \tag{3}$$

- For transverse modes:

$$f(C_{ij})=C_{44}\ \text{(a)},\ f(C_{ij})=0.5(C_{11}-C_{12})\ \text{(b)},\ f(C_{ij})=(C_{11}-C_{12}+C_{44})/3\ .\ \text{(c)} \tag{4}$$

The relevance of these elasticity-related features for a number of effects characteristics of coherent epitaxial solids and for epitaxy-induced structural phase transformations has been discussed in refs. [3,4]. In our approach, we derive renormalized expressions $-n_S-$ of the geometric factor n_1 showing the effect of the ratio S of the $S_{A,B}$ factors (effective elastic constants) of the substrate and the epilayer in the case of B/A heterostructur involving one interface. The relevance of S is depicted on Fig.1 for several heterostructures including nitrides-based systems. One can see that the highest values of n_S, i.e., the smallest MD's densities are obtained for S≅1 and that n_S decreases when the mismatch of the S_A and S_B factors increases.

For systems where a large lattice mismatch exists between the host materials, the strategy of growing buffer layers before the elaboration of the final overlayer is currently widely used. These transitional layers are aimed at ensuring a continuous matching of the relevant features of the host materials (substrate and overlayer) selected for the growth experiment. It is then important to develop reliable and well-based criteria in order to make an optimized choice of the buffer layer. These criteria are formulated by the continuity conditions for geometric (n_S) and elastic factors (S).



The epitaxial growth of GaN by modern growth techniques as metalorganic chemical vapor deposition is usually made by using sapphire as substrate. Despite the large lattice mismatch between these two materials (> 12 %), which implies, in principle, that a high density of dislocations may be present in the epilayer, it has been demonstrated that devices showing surprisingly high performance may be obtained. Defects which could damage the interface quality of the heterostructure are related to the existence of interface defects between misoriented domains in the GaN overlayer, consisting in low-angle grain boundaries. An alternative to the use of sapphire substrates can be provided by SiC, which affords a better lattice matching and closer thermal expansion properties. This is expected to give less stressed heterointerfaces and smaller extended defect densities and, consequently, improved crystalline characteristics. This improvement is indeed necessary to obtain high quality devices. One possible strategy to increase this crystalline quality is to introduce a buffer layer between the overlayer and the substrate. From this point of view,the choice of AlN as a buffer layer material is interesting because of the low lattice mismatch between AlN and SiC (≅ 1 %), while the thermal expansion coefficients of these materials are respectively $6.2x10^{-6}$ °K^{-1} and $4.3x10^{-6}$ °K^{-1}. Whe demonstrate that, when AlN is used as a buffer layer, the matching at the AlN/SiC interface, of the dynamics-strain related factors is improved. These theoretical previsions contribute to show that the SiC-substrate alternative with the use of AlN, instead of sapphire, is a valuable approach for GaN heteroepitaxy.

References

[1] See, e. g., J. W. Matthews, *Epitaxial Growth*, Part B (New-York, Academic, 1975) p. 505.
[2] See, e. G., C. Kittel, in Introduction to Solid State Physics, 3rd ed., Edited by J. Wiley and sons (New-York, 1968);p. 119.
[3] A. Zunger and D. M. Wood, J. Cryst. Growth, 98 (1989) 1.
[4] S. Froyen, Su-Huai Wei, and A. Zunger, Phys. Rev. B 38 (1988) 10124.